1-Butanol, 3-methoxy-3-methyl-, acetate

103429-90-9	DTXSID30145852

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.14

Global applicability domain: Inside

Local applicability domain index: 5.64e-01

Confidence level: 5.90e-01

Nearest Neighbors from the Training Set

Image not found

Methyl pivalate Measured: 1.83 Predicted: 1.76 Image not found

Paraldehyde Measured: 0.67 Predicted: 8.50e-01 Image not found

Ethyl orthoformate Measured: 1.20 Predicted: 1.05

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2-(Hexyloxy)ethanol Measured: 1.86 Predicted: 1.74 Image not found

Metaldehyde acetaldehyde

tetramer

Measured: 0.12 Predicted: 4.47e-01